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Final Technical Report

ONR Contract N00014-87-K-0481

Part 1. Mechanics of Thin Films; Part 2. Fracture of Solids

to

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May 28, 1991

Research Objectives

During the course of this project, research has been pursued along two distinct paths, consistent with the aims of the program outlined in the original proposal. The larger thrust has focussed on issues in the fabrication and processing of thin film materials for application in microelectronics, mainly the mechanics of defects in semiconductor materials. A second thrust has focussed on fracture of structural materials.

In the area of thin films, research has been concerned with the role of mechanical stress in defect nucleation and motion in strained, artificially structured materials. The simplest and most common configurati of this kind is a thin single crystal layer grown epitaxially onto a substrate under circumstances where the lattice parameter of the layer material differs from that of the substrate. The induced layer strain can be used to tailor electronic properties of the material but, on the other hand, the internal stress corresponding to this strain provides a driving force for nucleation and growth of crystalline defects, mainly dislocations and stacking faults. Such defects seriously degrade the performance of heteroepitaxially grown semiconductor films. The evolution of a defect distribution is intimately connected to the processing history of the material. Specific studies pursued have been:

(a) The conditions under which it first becomes energetically possible to introduce misfit dislocations at the interface between a strained layer and its substrate were established two decades ago. The criterion was expressed in terms of the behavior of a single, isolated dislocation extending from the free surface of the layer to the layer-substrate interface, the so-called threading dislocation. While the theory does indeed agree with the observed onset of interface misfit dislocation formation, it fails to provide a satisfactory description of elastic strain relaxation due to glide of numerous dislocations. Among the possible reasons for this difference are that dislocation mobility is low in semiconductor materials so that the process may be kinetically limited, or that the motion of a dislocation on any particular glide plane in the layer can be influenced by the presence of dislocations on other glide planes so that glide is retarded due to this interaction. One goal has been to understand the role of these effects in the strain relaxation process.

(b) One of the promising methods of thin film growth being developed at Brown is a form of solid-state epitaxy (known as solid phase epitaxy or SPE) of amorphous alloys on crystalline substrates. This particular growth process is of vital interest for integrated circuit device processing since the introduction of electronic dopants by ion implantation results in the damage and ultimate amorphization of the semiconductor near-surface region which must be regrown by the process of SPE. The particular case of solid phase epitaxy of strained $Si_{1-x}Ge_x$ is of ever increasing importance due to recent demonstrations of high speed heterojunction bipolar devices fabricated in this material. The principal goal of our research has been the application, extension and development of criteria for predicting strained-layer heteroepitaxial thin film failure.

Research on fracture mechanics applied to structural materials was focussed on the following issues:

(c) It has been observed that if a steel plate containing an edge crack is struck by a projectile on one side of the crack mouth then fracture can be initiated in either of two modes, depending on the impact velocity and material velocity. In one case, the crack will grow as a tensile crack in a direction oblique to the original crack, whereas under other conditions the crack will grow straight ahead as a shear crack. The difference is important in applications where fracture initiation and fragmentation must be predicted under impact loading conditions. A fracture mechanics analysis of this process has been undertaken in order to establish the discriminating conditions between the two fracture modes.

(d) Motivated by the role of embedded fibers in increasing the fracture toughness of brittle materials, a study has been recently started on the process of sliding of a fiber through an elastic matrix. It has been observed that if a crack advances through a brittle fiber-reinforced material, the crack front in the matrix leaves in its wake unfractured fibers bridging the gap between the crack faces. These fibers can increase the fracture toughness of the composite material by dissipating energy as they are pulled out of the material to complete the fracture process. The goal is to understand the mechanics of the pull out process and its influence on fracture resistance.

Principal Results

Modeling of defects in strained epitaxial layers

With reference to goal (a), a general definition of driving force for glide of a threading dislocation in a strained layer was introduced on the basis of work arguments. The definition was then applied to calculate the driving force for steady motion of an isolated threading dislocation in a strained layer, and it was shown that the result includes Matthew's critical thickness concept as one of its features. Next, a kinetic equation for glide of a dislocation in semiconductor materials was proposed to estimate the glide rate of a threading dislocation in these low mobility materials, with the predicted glide rates being in good agreement with observed rates in SiGe alloys at elevated temperatures.

As noted above, in a strained layer grown epitaxially on a substrate, the motion of a dislocation on any particular glide plane in the layer can be influenced by the presence of dislocations on other glide planes. To obtain quantitative estimates of this interaction for strain relaxation in an epitaxial layer, the general definition of driving force for glide of a threading dislocation in a nonuniform stress field was adopted to calculate the driving force on a threading dislocation due to an encounter with an interface misfit dislocation on an intersecting glide plane; see Fig. 1. The result was examined in detail for the case of cubic materials, taking into account different combinations of Burgers vectors. The analysis makes it clear that the misfit dislocation forces the threading dislocation to glide through a channel of width less than the full layer thickness. A blocking criterion in terms of mismatch strain ϵ_0 and ratio of film thickness to Burgers vector h/b was proposed, based on the presumption that blocking will occur if the channel width is less than the critical thickness for the local reduced strain. The results shown in Fig. 2 indicate that this effect can be significant in blocking the glide of a threading dislocation, depending on the mismatch strain magnitude and the layer thickness.

The application of the strain energy concept to the determination of critical thickness in Ge-implanted Si was demonstrated. To do this a number of considerations were applied: (i) stacking faults rather than 60° dislocations are the kinetically favored defect for strain relief during solid phase epitaxy, (ii) there is no well defined compositional interface in ion implantation synthesized layers, and (iii) the analysis must take into account the variations in layer stresses through the thickness of the thin film. In the analysis of critical thickness effects associated with compositionally abrupt interfaces (i.e. materials synthesized by MBE or CVD), the strain relieving 60° misfit dislocations lie at the substrate/strained-layer interface. In the case of Ge-ion-implanted-Si, however, the composition varies with a Gaussian profile through the thickness of the layer. Under these conditions the stable position of a defect must be found by determining the position in the film where the forces acting on the defect are balanced. Fig. 3a shows schematically a dislocation lying on its glide plane (inclined a degrees from the vertical) at a depth y from the surface. The forces which act to move the dislocation along the glide plane are an image force F_{im} which tends to pull the defect toward the surface, the force F_{sf} due to stacking fault energy which tends to pull the bounding partial dislocation along the glide plane toward the surface, and the Peach-Koehler glide force F_{pk} due to lattice mismatch tending to push the dislocation into the substrate. The forces on the defect will be balanced at that depth from the surface where $F_{im} + F_{sf} = F_{pk}$. This is shown schematically in Fig. 3b.

Experimental observations on electronic materials

Both the presence of defects and the development of the a/c (amorphous/crystalline) interface microstructure during solid phase epitaxy of ion implantation-synthesized $Si_{1-x}Ge_x$ were established with cross-sectional transmission electron microscopy. Micrographs were obtained which show the a/c-interface in the as-implanted condition and after 50, 300, and 600 s at 590°C. Representative examples of cross-sectional TEM micrographs from a $Si_{1-x}Ge_x$ (x=14 at. %) alloy are presented in Fig. 4a-d. The as-implanted microstructure, shown in Fig. 4a, consists of a uniformly amorphous region that extends 340 nm from the surface into the wafer. Although not visible in Fig. 4a, Rutherford Backscattering Spectroscopy results establish that the peak of the Ge implant is at a depth of 130 nm from the surface. Similar TEM results were obtained from samples with alloy compositions of 3, 7, and 13 at.%. which showed that the 3 and 7 at. % alloys were defect-free, while the 13 at. % samples were densely populated with planar defects such as stacking faults and microstwins and hence were unsuitable for device applications. These experimental results are consistent with our calculated critical implant dose at 200 keV of 10 at. % Ge. Thus, we have demonstrated, experimentally, the utility of our modifications to the critical thickness theory.

Fracture of solids

Concerning goal (c) above, the two dimensional elastodynamic problem of a semi-infinite plate containing an edge crack has been considered. Initially, the plate is stress free and at rest. To simulate the asymmetric impact of a projectile on the cracked edge of the plate, a normal velocity is suddenly imposed on the boundary of the plate on one side of the edge crack. The boundary of the plate and the crack faces are otherwise traction free. Due to the nature of the loading, a combination of transient mode I and mode II deformation fields is induced near the crack tip. The corresponding stress intensity factor histories have been determined exactly for the time interval from initial loading until the first wave scattered at the crack tip is reflected at the plate edge and returns to the crack tip. In experiments on fracture initiation in a high strength steel based on essentially this specimen and loading configuration, Kalthoff and Winkler (in *Impact '87*, 1987) reported a fracture grew from the original crack either as a tensile crack inclined to the original crack plane or as a straight ahead shear fracture , depending on the intensity of the applied velocity. The elastodynamic analysis appeared to capture the essence of the experimental observations for tensile crack growth. To study the influence of high strain rate plasticity in initiating the adiabatic shear band in this model, a large scale numerical simulation of the crack tip region was carried out, including the features of strain hardening, thermal softening, and strain rate sensitivity. Both brittle and ductile fracture criteria were assumed, with the mode of fracture initiation being determined by whichever criterion could be satisfied first in time. The numerical results showed the same type of fracture mode conversion as observed in the experiments.

Some exciting new results on the fiber pull out problem have resulted from a study initiated only recently, in connection with assessing the fracture toughness of fiber-reinforced composite materials. The process of sliding of a circular elastic fiber through a hole in an otherwise unbounded elastic matrix has been modeled. The fiber interacts with the surrounding matrix material through Coulomb friction on its lateral faces. An axial force is applied to one end of the fiber, and the other end is free of traction. Exact asymptotic solutions are obtained for the cases when the fiber is very stiff or very compliant compared to the matrix material, and numerical results are obtained to describe the transition between these two extreme cases. It is shown that, for a long fiber, the total force needed to slide the fiber against frictional resistance is independent of the length of the fiber and of the coefficient of friction. The reason for this outcome is that the frictional resistance to sliding is localized to some portion of the fiber near its free end. The rate of decay of the localized effect, which is represented by an exponential decay parameter, depends on several factors. If the matrix and fiber materials are the same and the coefficient of friction is one-half, then the characteristic exponential decay length is about ten fiber diameters.

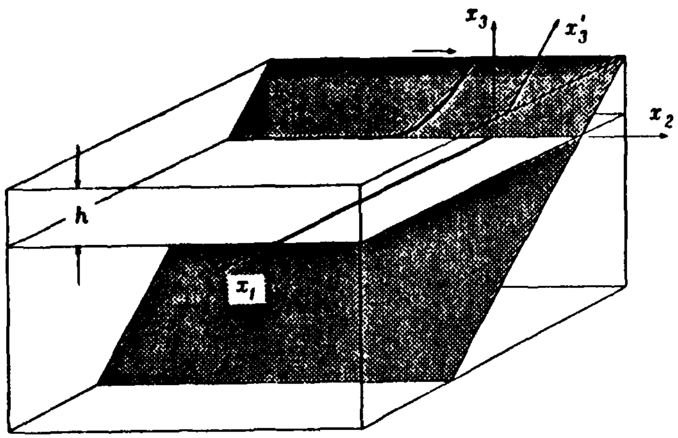
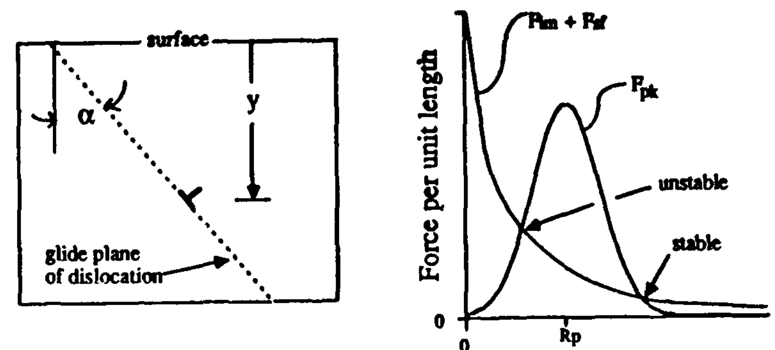


Figure 1



Defect position on glide plane

Figure 3

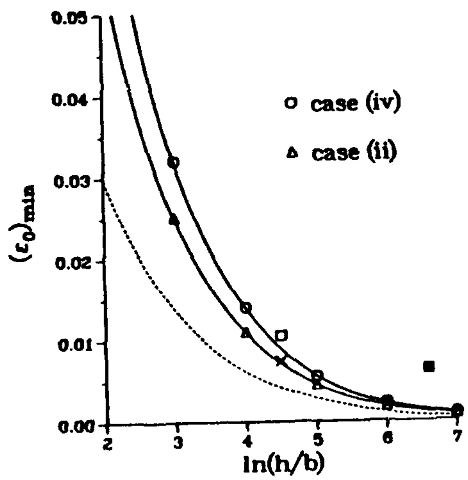


Figure 2

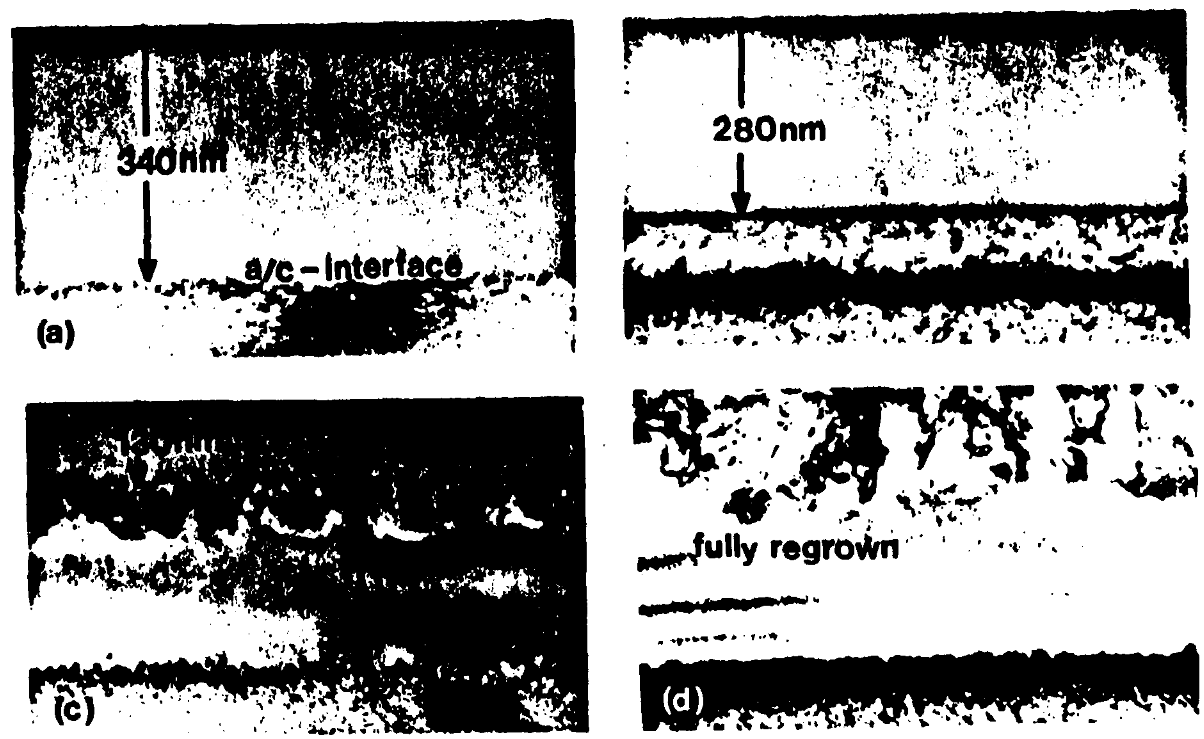


Figure 4

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